X-Ray Studies of Superlattice Ordering in $(Pb(Mg_{1/3}Nb_{2/3})O_3)_{0.9375}(PbTiO_3)_{0.0625}$ Relaxor

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Introduction: $(Pb(Mg_{1/3}Nb_{2/3})O_3)_{0.9375}(PbTiO_3)_{0.0625}$ (PMN-6.25%PT) belongs to a special class of ferroelectric relaxor materials. It doesn't undergo any macroscopic structural phase transition, but local order was suggested to deviate from average cubic in the nano-size regions. Studies of superlattice short-range ordering in these regions are expected to help us better understand the structure-properties relationship in relaxors.

Methods and Materials: Single crystal of PMN-6.25%PT in the shape of parallelepiped had linear dimensions of 5x5x0.5 mm^3 and surface normal in [001] direction. Energy of the x-rays was tuned to 10 keV. Studies of the superlattice short-range order peaks were done in the reflection geometry on the sample enclosed in the closed cycle He compressed gas cryostat in the 15-300 K temperature range. Cryostat was mounted on the four circle Huber single crystal diffractometer.

Results: Two types of short-range order superlattice peaks have been found: a) F peaks and b) α peaks (see Figure 1). The main contribution to the F peaks is coming from the Nb/Mg chemical short-range ordering in [111] direction. These F peaks show very weak temperature dependence and the size of the ordered regions of 24 Å was determined from the width of these reflections. Without Ti doping in pure $Pb(Mg_{1/3}Nb_{2/3})O_3$ (PMN) the size of the chemically ordered regions was found to be about 50 Å. Integrated intensity of the weak superlattice reflections (α peaks), which originate from [011] type ordering, was found to be temperature independent between 15-100 K. The integrated intensity above 100 K was gradually decreasing with temperature in the linear fashion. The interpolation of the integrated intensity to zero was near T_f=260 K. This interpolated temperature marks the local structural phase transition in the regions of about 31 Å in size. The size of these regions was found to be temperature independent within the experimental errors. The origin of the α peaks is attributed to the oxygen octahedra rotations. Correlation radius of 31 Å is very similar to the one for pure PMN, but interpolation of the integrated intensity of the α peaks in pure PMN to zero was found near T_f=220 K, rather than at 260 K in the composition under study.

Conclusions: PMN-6.25%PT doesn't' undergo any macroscopic structural phase transition and the average structure, derived from fundamental Bragg reflections, is cubic in the whole temperature interval. Interpolated 260 K temperature of the disappearance of the α superlattice peaks marks the local structural phase transition in the regions of 31 Å. The temperature of this local phase transition is close to the temperature where the maximum of the dielectric constant occurs when the frequency of the applied AC electric field is approaching the zero. Similar conclusion can be made for pure PMN with the interpolated transition temperature of 220 K. Therefore the studies of the phase transition from the superlattice reflections may help us better understand the structrure-properties relationship in the ferroelectric relaxors. Studies of PMN with other concentrations of Ti doping are underway.

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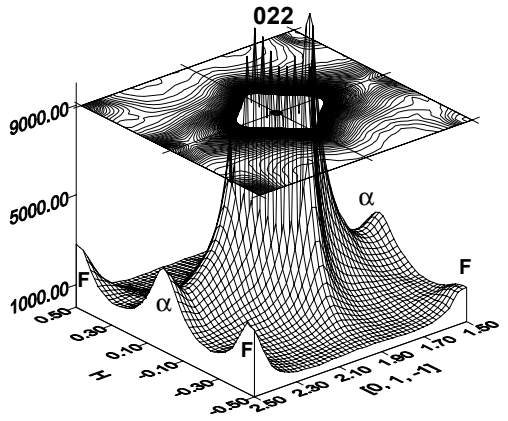

Figure 1. Section of the reciprocal space near (022) Bragg peak with F and α superlattice peaks in PMN-6.25%PT at 15 K